Numerical Simulation of Particle Focusing Dynamics of DNA-Laden Fluids in a Microtube

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Abstract

A CFD model considering inertial, elastic and drag forces was developed to simulate the focusing effect of microparticles in a dilute DNA solution passing through a microtube. The Oldroyd-B fluid model coupled with the Lagrangian model was employed to describe the flow behavior of DNA solution and particle trajectory. The model was validated by comparing the patterns of particle beam and its width with experimental results. Particle focusing dynamics was investigated by analyzing the focusing behaviors, flow and particle velocity, and force distributions throughout the whole tube. The results indicated that particles far away from the centerline migrate faster than those near the centerline. Investigations on the effect of DNA concentration, particle diameter and flow rate showed that increasing DNA concentration and particle diameter benefited the focusing efficiency while larger flow rate worsened the particle focusing. This computational model could serve as an effective tool to investigate the particle focusing dynamics.

Key Words: Particle focusing; DNA-laden fluid; Microfluidics; CFD simulation; Microparticle manipulation

1. Introduction

Particle migration is a vital issue in suspensions for a wide range of engineering applications such as transport of sediments (*Merkak et al, 2009*), oil recovery *(Sharma et al., 1987*), heat transfer (*Molerus et al., 1995; Bahiraei et al., 2015*), composite materials (*Yuan et al., 2015*), coating process (*Ritz et al., 2000*), sequestration process (*Xie et al., 2017*), separation or mixing process (*Ahn et al., 2015: Lin et al., 2018*). With the fast growth of microfluidic devices in recent years, significant research has been conducted to study the migration effects of particles suspended in a flowing liquid that are strongly enhanced in a highly confined system (*Ahn et al., 2015; D'Avino et al., 2017*). The confinement effects from microchannels provide a sufficient driving force for a particle to migrate across streamlines, enabling passive manipulation of a particle in both Newtonian (*Godin et al., 2008; Xuan et al., 2010*) or non-Newtonian fluid (*Leal et al., 1979; McKinley et al., 2002*). This phenomenon of cross-streamline migration is essential for particle manipulation in a variety of chemical, biological and environmental applications, for instance, particle fabrication, flow cytometry, biomedical diagnosis and cell-sorting (*Xuan et al, 2010; Hur et al., 2010; Dannhauser et al., 2014*).

Particle focusing as one of the most obvious applications of particle migration is often a necessary step prior to sorting, counting, detecting and analyzing particles in flow cytometers or continuous-flow sorters (*Lu et al., 2017*). Many researchers concentrated on the focusing effect of particles in Newtonian fluids in a microchannel, where the cross streamline migration was mainly caused by inertial forces. (*Carlo et*

al., 2007; Masaeli et al., 2012; Oakey et al., 2010). However, multiple equilibrium positions in a Newtonian medium may hinder the achievement of single line particle focusing. A more effective focusing method to overcome the above problem is highly desired. The methods currently in use, including active focusing and passive focusing, require either external force fields or auxiliary streams. Those techniques, however, need additional components or complicate channel geometries, consequently increasing fabrication complexity and costs. Therefore, many researchers have recently paid attention to elastic effects in viscoelastic fluids (*Ahn et al., 2015; Song et al., 2016; Cha et al., 2014; Yang et al., 2012*). Due to the non-uniform distribution of the first normal stress difference of a non-Newtonian fluid, particles tend to be driven away from walls and migrate toward the centerline of microchannels (*Leshansky et al., 2007*). However, the throughputs of such techniques may be restricted by a narrow range of flow rates.

Owing to much longer relaxation time, DNA solutions possess much higher elasticity than synthetic polymer solutions, enabling a more effective particle focusing at a larger flow rate (*Kang et al., 2013*). Kang et al. (*2013*) demonstrated for the first time a highly tunable particle focusing method over a wide range of flow rates by using a DNA-laden fluid. The use of DNA-laden fluid could achieve a significantly high elastic number at low viscosities, therefore, can be utilized in a wide range of applications. It was also claimed that this method could open up a new way to quantitatively detect the very weak non-Newtonian elastic properties of low viscosity biopolymer solutions (*Kang et al., 2013; Bhat et al., 2010; Brust et al., 2013*). A comprehensive investigation on the particle dynamics and focusing efficiency for the

DNA-laden fluid in microchannels is therefore of great significance.

Factors affecting the migration of particles, such as parameters related to inertia, elasticity, blockage ratio, and shear thinning, have been investigated by several researchers (*Villone et al., 2011; D'Avino et al., 2012; 2019; Lim et al., 2014a; Seo et al., 2014; Lim et al., 2014b; Giudice et al., 2015*). Despite the above studies, the mechanisms of particle focusing caused by the combined effects of fluids properties, particle-fluid interaction and flow conditions are not clarified. Although numerical simulation could provide detailed information compared to experimental studies, most of the previous numerical studies considered either sole elastic effect or sole inertial effect based on a steady-state assumption. None of the previous works on particle focusing have been able to accurately predict the transient particle concentration distribution measured over a range of operating conditions for DNA suspension system. Comprehensive numerical studies taking into account both elastic and inertial effects on the system with DNA solution in microchannels have not been reported so far. Particle focusing dynamics in DNA-laden fluid in microchannels still needs to be investigated thoroughly, requiring a transient model to capture the detailed information of particle motion.

In this study, a CFD model based on the Lagrangian approach was developed to investigate the particle focusing dynamics in a DNA-laden fluid flowing through a microtube. Inertial force, elastic force and drag force were all considered and incorporated into the model. The transient migration behavior of particles in dilute DNA solution was investigated by the developed model which was less explored previously.

Effects of DNA concentration, particle diameter and fluid flow rate on the particle focusing dynamics and efficiency were studied based on the developed CFD model.

2. Physical models and mathematical formulations

2.1. Problem description

The particle focusing experimental system presented in Kang et al's work (*Kang et al., 2013*) was selected as the studying object to validate the developed CFD model in this work. Briefly, particles in a DNA solution was pumped through a silica microtube. The particles used in the particle focusing study are polystyrene (PS) microspheres with diameters of 5.8 μm and number densities of 9700 μl^{-1} in the suspension. λ-DNA which has relatively long relaxing time and a low overlapping polymer concentration is used to prepare DNA solution with a concentration of 5ppm as the carrying medium. The solvent used is TBE buffer solution with 22wt% glycerin. The silica microtube coated with polymer is with a diameter of 50 μm and length of 5 cm. The flow rate was controlled by syringe pumps (11 Plus, Harvard Apparatus). The particle dynamics were characterized by optical microscopes (BX60, Olympus) and high-speed camera (Fastcam MC2, Photron). According to the experiment mentioned above, the simulation was carried out in a 2D microtube with a diameter of 50 μm and length of 5 cm. Since glycerin was added to adjust the density of the solution to eliminate particle sedimentation in the experiment, buoyancy and gravity were not considered in this study. The details of model parameters and operating conditions were listed in **Tables 1-2**.

2.2. Governing equations for DNA solution

DNA solution exhibits both viscous and elastic behavior under stain. Since the viscosity almost keeps constant at the low concentration of DNA, the fluid of DNA solution in this work is treated as Oldroyd-B fluid and incompressible with a constant density. The mass conservation can be expressed as:

$$\nabla \cdot \vec{v} = 0 \tag{1}$$

where $\vec{v}$ is the velocity of fluid.

The Oldroyd-B fluid model is used to describe the viscoelastic behavior of the DNA solution. The momentum equation can be expressed as follow:

$$\rho\left(\frac{\partial \vec{v}}{\partial t} + \vec{v} \cdot \nabla \vec{v}\right) = \nabla \cdot \underline{\underline{\sigma}} \tag{2}$$

$\underline{\underline{\sigma}}$ is the total stress which can be presented as:

$$\underline{\underline{\sigma}} = -p\underline{\underline{I}} + \eta_s[\nabla \vec{v} + (\nabla \vec{v})^T] + \underline{\underline{T}} \tag{3}$$

where η_s is the viscosity of solvent and $\underline{\underline{T}}$ is extra stress contributed by the DNA. The constitutive relation can be expressed as:

$$\underline{\underline{T}} + \lambda \frac{D\underline{\underline{T}}}{Dt} = \eta_p[\nabla \vec{v} + (\nabla \vec{v})^T] \tag{4}$$

where λ is the relaxation time of DNA and η_p is the viscosity contributed by DNA. The upper convective derivative operator is defined as:

$$\frac{D\underline{\underline{T}}}{Dt} = \frac{\partial \vec{v}}{\partial t} + (\vec{v} \cdot \nabla)\underline{\underline{T}} - [(\nabla \vec{v}) \cdot \underline{\underline{T}} + \underline{\underline{T}} \cdot (\nabla \vec{v})^T] \tag{5}$$

And the total viscosity of the solution is defined as:

$$\eta = \eta_p + \eta_s \tag{6}$$

The Weissenberg number (*Wi*), Reynolds number (*Re*) and elasticity number (*El*)

are three dimensionless parameters used to characterize the nonlinear forces generated in viscoelastic fluids. Weissenberg number (*Wi*) representing the relative of elastic force to viscous force is defined as (*Nam et al., 2012*):

$$Wi = \lambda \frac{U}{R} \tag{7}$$

where U and R are the average fluid velocity at the inlet and the radius of the microchannel.

The intrinsic nonlinear inertial effect leads to particle migrating across the streamline. Reynolds number (*Re*) is used to quantify the relative magnitude of viscous and inertial effects, which can be expressed by the ratio of inertial force to viscous force (*Nam et al., 2012*):

$$Re = \frac{\rho DU}{\eta} \tag{8}$$

where ρ is the solution density, *D* is the hydraulic diameter of microchannel.

In a DNA solution, the inertial and elastic forces acted on the particle synergistically. The relative magnitude of inertial force and viscous force can be quantified via the elasticity number (*El*):

$$El = \frac{Wi}{Re} \tag{9}$$

With the dimensionless parameters, the non-dimensional formulation for the DNA solution can be expressed by the following:

$$\nabla \cdot \vec{v} = 0 \tag{10}$$

$$Re\left(\frac{\partial \vec{v}}{\partial t} + \vec{v} \cdot \nabla \vec{v}\right) = \nabla \cdot (-p\underline{\underline{I}} + \mu_s[\nabla \vec{v} + (\nabla \vec{v})^T] + \underline{\underline{T}}) \tag{11}$$

$$\underline{\underline{T}} + Wi(\frac{\partial \vec{v}}{\partial t} + (\vec{v} \cdot \nabla)\underline{\underline{T}} - [(\nabla \vec{v}) \cdot \underline{\underline{T}} + \underline{\underline{T}} \cdot (\nabla \vec{v})^T]) = \mu_p[\nabla \vec{v} + (\nabla \vec{v})^T] \tag{12}$$

where μ_s and μ_p are the relative viscosities of the solvent and polymer, respectively.

$$\mu_s = \frac{\eta_s}{\eta} \tag{13}$$

$$\mu_p = \frac{\eta_p}{\eta} = 1 - \mu_s \tag{14}$$

2.3. Governing equations for particles

The motion of the particles is governed by the following force balance based on Newton's second law:

$$\rho_p(\frac{\pi}{6}d_p^3)\frac{d\vec{u}}{dt} = \vec{F}_T \tag{15}$$

where ρ_p is the density of particles in suspension, d_p is the particle diameter and $\vec{F}_T$ denotes the total force exerted on the particle.

Attributed to the shear stress and pressure acting on the particle surface, a force is exerted on the particle when a viscoelastic fluid flowing past it. This force can be decomposed into two components, namely, lift and drag. The induced lift force in a DNA solution flow is one of the main force driving the cross-stream motion of particles. This force can be further broken down into two forces which are the inertial lift (F_{iL}) due to fluid inertia and the elastic lift (F_{eL}) due to fluid elasticity.

The inertial lift force consisting of wall-induced and shear gradient induced inertial lifts can be expressed as follow:

$$F_{iL} = F_{iLw} + F_{iLs} = C_{iL}\rho d_p^4 \dot{\gamma}^2 \tag{16}$$

The elastic lift force exerting on a particle is caused by the non-uniform normal stress differences in viscoelastic fluid flows. As the magnitude of second normal stress is much smaller than that of first normal stress difference for the most viscoelastic

solutions, the elastic lift force can be expressed by (*Leshansky et al., 2007*)

$$\vec{F}_{eL} = C_{eL} d_p^3 \nabla N_1 \quad (17)$$

where C_{eL} is the non-dimensional elastic lift coefficient, and N_1 is the first normal stress difference.

$$N_1 = T_{11} - T_{22} = -2\eta_p \lambda \dot{\gamma}^2 \quad (18)$$

where T_{11} and T_{22} are the normal stresses in the translational direction and velocity gradient direction, respectively.

The drag force exerted on the particle in this system can be calculated using the following equation:

$$\vec{F}_D = \frac{1}{8} C_D (\pi d_p^2) \rho |\vec{u} - \vec{v}| (\vec{u} - \vec{v}) \quad (19)$$

where C_D and ρ are the drag coefficient and fluid density, respectively.

2.4. Modeling strategies

A transient Laminar flow coupled with a Lagrangian model was used to simulate the flow behavior and describe the particle dynamics. It was reported that the viscosity contributed by polymer was corresponded to $\eta_s c[\eta]$ for a dilute polymer solution (*Tirtaatmadja et al., 2006; Kang et al., 2013*), where $[\eta]$ is the intrinsic viscosity of polymer solution and *c* denotes the polymer concentration. It was also reported by Graessley (*1980*) that the intrinsic viscosity can be correlated with the overlapping concentration c^* by $[\eta] = 0.77/c^*$. Therefore, the viscosity contributed by DNA η_p was corresponded to $0.77\eta_s c_{DNA}/c^*$ in this study. The Lagrangian model based on Newton's laws of motion consisting of equations (15)-(19) was solved to obtain the

position and velocity of discrete particles over time. The inertial lift force due to fluid inertia and the elastic lift force were incorporated into the particle momentum equation as source terms. The motion of the particles also imposes a force on the fluid and affects the flow domain (*Leighton et al., 1987; Phillips et al., 1991*). However, the exact momentum force on the fluid induced by particle motion cannot be implemented directly in equation (2) for the simulation framework in the present study since the position of the particles at the any given instant is between the mesh nodes. Therefore, the momentum force imposed on the fluid was calculated by $\vec{F}=\vec{F}_D/V_{mesh}$ and then smeared over the mesh element corresponding to the particle location. V_{mesh} is the volume of a mesh element.

The physical properties of the materials and the operating conditions used were summarized in **Table 1**. The simulation was performed based on a finite element method in COMSOL software. A 2D rectangular geometry with a width of a 50 μm, length of 5 cm and mesh number of 100,000 was constructed as the computational domain. Note that half of the 2D domain may be sufficient if the geometry is axisymmetric and the external forces are isotropic. In this study, considering the model applicability for more complex geometry of microchannels in our follow-up study, the model was developed based on a full 2D geometry. It can benefit the transfer of the present model to non-axisymmetric systems. The coordinate origin located at the midpoint of the left side edge of the rectangle which was also the inlet of the microtube. The right side edge was defined as an outlet and the other boundaries were defined as a wall. The details of boundary conditions were shown in **Table 2**. Since the particle

focusing pattern reaches steady state after t = 40 s, the simulation results were analyzed by taken time-average from t = 40 s to 50 s in the following sections unless specifically mentioned.

3. Results and Discussion

3.1. Model validation

The developed model was first validated qualitatively by comparing the simulated particle stream pattern with experimental results. The CFD simulation was conducted at the same conditions used in the experiment (*Kang et al., 2013*). In short, a 5 ppm DNA solution containing particles (1050 kg/m^3 in density and 5.8 μm in diameter) was introduced into a 50 um diameter tube at a flow rate of 10 μl/h. **Figure 1(a)** shows the particle stream distributions at various axial positions. **Figure 1(b**) gives the simulated results of stacked particle trajectories colored by the value of radial positions (Y-direction) at the corresponding axial positions (X-direction) when t = 50 s. According to the particle stream patterns shown in **Figure 1**, the prediction by developed CFD model (**Figure 1(b)**) agrees well with the experimental observation (**Figure 1(a)**). For both experimental observation and simulated results, the development of particle beams displays similar trends. The particle beams become narrower and narrower in width along the axial direction.

Quantitative validation was further conducted by comparing the predicted half-width of particle stream with experimental results (**Figure 2**). The simulation data was obtained by doing time-average from t = 40 s to 50 s. The experimental data was

obtained by measuring the quantity of interest in the stacked microscopic images of particle stream (**Figure 1(a)**) via Image J. In order to eliminate the noise in experimental images, $y_{99\%}$, defined as the half-width of particle stream within which 99% of particles are located around the centerline, was used as the quantity of interest for comparison. First, the width of the particle stream (also named as particle beam) at the four locations of microtube was obtained by measuring at least 10 different positions for each sub-image shown in **Figure 1(a)**. The average value of the measured widths of the particle stream was then divided by two to get the half-width of particle stream. As shown in **Figure 2**, the simulated data and experimental measurement are in pretty good agreement, further confirming the availability of the developed model in this study.

3.2. Model applications

3.2.1. Flow behaviors

The flow behaviors of DNA solution in the microtube were studied to understand the particle lateral migration mechanism. **Figure 3** gives the flow velocity distributions at different sections of the microtube. In this case, the velocity of DNA solution at tube inlet is set as 1.42×10^{-3} m/s according to the flow rate and the entrance length L is calculated to be 1.06×10^{-7} m according to the equation $L/D = 0.06Re$. As shown in **Figure 3**, the smallest flow velocity magnitude can be seen in the region near the tube-wall. The flow velocity increases along the direction from the wall toward the centerline of the tube. The maximum flow velocity reaches 2.12×10^{-3} m/s appearing at the centerline. The shear gradient increases from centerline to wall according to the velocity

profile, suggesting that particles may migrate from centerline to the tube wall. However, particles focus effectively toward the centerline as shown in **Figures 1-2**, implying that the inertial lift force is not dominant for the particle migration and have little effect on the particle focusing in this case. More details regarding the effect of inertial force on the particle motion in this study are discussed in the later section. It is also noted that the distributions of flow velocity at different sections of microtube display similar patterns (**Figure 3(A)**). The radial distribution of flow velocity at the axial position from X = 0 to X = 0.0499 m almost keeps the same pattern (**Figure 3(B)**). Only a slight difference can be observed at the outlet of the tube (X = 0.05 m). This difference could be caused by the use of pressure-out as the outlet boundary condition. Papanastasiou Open Boundary Condition (*Dimakopoulos et al., 2009; 2012*) is suggested to further improve the present model. Although there may be certain deviation occurring at the outlet region in this study, the present model could predict particle focusing effect precisely for main portions of the computational domain where good agreement between simulation results and experimental data was obtained (**Figures 1-2**).

3.2.2. Dynamics of particle focusing

3.2.2.1. Particle focusing behaviors

In order to get insights into the focusing behaviors in such system, particle distributions in the microtube were analyzed after t = 40 s when the flow reaches steady-state. **Figure 4** shows the radial particle distributions at various axial positions. At the inlet of the microchannel (X = 0 m), the particle was assumed to be uniformly

distributed in this study. At the axial position of 0.1 cm away from the inlet, particle fractions exhibit higher values at the radial position (Y-direction) within the ranges of 17.5 ~ 22.5 μm and -17.5 ~ -22.5 μm as compared to the other radial positions. In contrast, fewer particles appear at the vicinity of the tube wall. This implies that the particles near the wall migrate across the streamlines toward the centerline and locate at the regions between 0.7 ~ 0.9 of the half-width of the tube. At the position near the middle of microchannel, particles only appear at the regions ±12.5 μm off-center distance and more than 25% of the particles are located at the region ±2.5 μm of the centerline, indicating that the particle stream becomes more focused at the center of the channel. At the tube outlet (X = 0.05 m), 100% of the particles concentrate within ±7.5 μm of the centerline. It is worth to note that the particle distribution does not follow a Gaussian distribution at when X ≤ 0.026 m. Instead, high particle concentrations can be observed not only at the centerline region but also at the vicinity of the boundaries of the particle beam. This implies that the particle lateral migration rate at different radial positions is not a constant value and those particles far away from the centerline may migrate faster than those near the centerline.

To further investigate the particle focusing dynamics, the plot of particle lateral position against time (t = 0 s to 35 s) for the particles with different initial positions is presented in **Figure 5**. As shown in **Figure 5**, the lateral position of particles decreases as the time proceeds. The decreasing rate of particle lateral position also displays monotonic decreasing relationship with time. This indicates that the lateral migration velocity of particle may be high at the position near the wall and becomes smaller and

smaller along the direction towards the centerline. In addition, it can be seen that particles initially located at the position far away from the centerline correspond to a larger slope of the y_p-t curve. Therefore, it can be concluded that particle with larger value of initial radial position will migrate faster towards the centerline than that with a smaller value. This also explains the reason why high particle concentrations can be observed not only at the centerline region but also at the vicinity of the boundaries of particle beam at the beginning of particle focusing process (**Figure 4)**.

3.2.2.2. Particle velocity

Based on the developed CFD model, the particle velocity throughout the whole microtube can be obtained. **Figure 6** gives the distributions of particle axial velocity in various regions of the microtube. As shown in **Figure 6(A)-(a)**, particles near the boundary of the particle beam have the lowest velocity while the highest velocity appears at the centerline. The particle axial velocity distribution follows a similar pattern with the flow velocity distribution (**Figure 3**). Due to the focusing effect of particles, the particle beam becomes narrower and narrower along the axial direction (X-direction) of the tube. The gradient of particle axial velocity along the radial direction (Y-direction) decreases (**Figure 6(A)-(B)**), indicating smaller discrepancy of particle axial velocity along Y-direction.

Figure 7 shows the distribution of particle lateral migration velocity (radial velocity). Positive velocity means that the particle travels upward while negative velocity represents the downward migration. As shown in **Figure 7**, particles above the

centerline are with negative radial velocity, indicating downward movements of these particles. In contrast, those below the centerline being with positive velocity move upward to the centerline. As compared to the particle axial velocity (~10^{-3} m/s), the magnitude of lateral migration velocity (~10^{-6} m/s) is approximately 3 order lower. It can be also found that the highest radial migration velocity appears at the boundaries of the particle beam and the velocity decreases with the decreasing distance to the centerline, further confirming the deduction from **Figures 4-5** in the previous sections. Different from the particle axial velocity shown in **Figure 6(B)**, **Figure 7(B)** shows that the particle radial velocity also changes along the axial direction of the tube. By comparing the distributions of particle radial velocity along Y-direction at the axial positions of X=0.001 m and X=0.025 m, it can be seen that the particle radial velocity increases along the axial direction. However, only a slight difference can be seen in the latter half of the tube when comparing the distribution of particle radial velocity at the position of X=0.025m with that at X=0.05m. The comparison of the radial velocity between particle and DNA solution (**Figure 8**) suggests that the lateral migration only occurs for the particles and the fluid radial velocity is almost close to zero.

3.2.2.3. Forces exerted on particles

Since the total force exerted on the particles governs the particle migrations, the various forces were analyzed in this section. It is also worth to note that the shear-induced migration of DNA molecules in the microtube would cause local inhomogeneity in the concentration and stress fields (*Tsouka et al., 2014; 2016*), which

may further affect the particle migration.

Figure 9 depicts the distribution of inertial force and elastic force at various axial (X-direction) and radial (Y-direction) positions of the microtube. Positive force represents the direction of force pointing upward. The inertial force and elastic force were calculated based on the flow field and particle properties according to Eq.(16) and Eq. (17), respectively. As shown in **Figure 9**, the elastic force points upward at the region below the centerline (Y<0). In contrast, positive inertial force appears at the region above the centerline (Y>0). Both forces have their highest values at the vicinity of the wall (Y = 25 μm) and decrease as the distance to centerline gets shorter. However, the maximum elastic force reaches ~1.2×10^{-13} N while the maximum inertial force is ~6.2×10^{-15} N. This indicates that the particle motion may be dominant by elastic force in this case where Re = 0.0338, Wi = 7.926 and El = 234.273. It can be also seen that both inertial force and elastic force display uniform distribution along the axial direction.

Figure 10 gives the elastic force acted on the particles. The colored region shown in **Figure 10(A)** was plotted by stacking 500 time-frames of particle trajectories and coloring them with the value of elastic force on the particles. The elastic force exerted on particle points upward at the region below the centerline (Y<0) while it points downward at the region above centerline (Y>0), driving particles to migrate toward the centerline of the tube. The outer particles around the centerline experience larger elastic forces, suggesting that particles far away from the centerline will migrate faster than those near the centerline. This is consistent with the conclusion obtained from the early

section (**Figure 7**). As shown in **Figure 10(B)**, the elastic force acted on particles exhibits almost a linear relationship with the Y-position. The force hardly changes along the X-direction at the range of -5 μm < Y < 5 μm.

Figure 11 depicts the inertial force acted on the particles during the focusing process. Similarly, the colored region shown in **Figure 11(A)** was plotted by stacking 500 time-frames of particle trajectories and coloring them with the value of inertial force on the particles. In contrast to the elastic force (**Figure 10**), the inertial force exerted on particle points downward at the region below the centerline (Y<0) while it points upward at the region above centerline (Y>0), which gives rise to particle lateral migration from centerline to wall of the tube. The outer particles around the centerline receive larger inertial force; however, the magnitude of the inertial force is much smaller than that of the elastic force. As shown in **Figure 11(B)**, at the axial position near the entrance (X = 0.001m), the inertial force acted on those particles in the region near the wall drops quickly as the distance to the centerline reduces. With the particle position getting closer to the centerline, the decreasing gradient of the inertial force becomes smaller. Although the overall trend of inertial force is different from that of the elastic force, both forces display slight differences along the X-direction in the range of -5 μm < Y < 5 μm.

Besides the elastic force and inertial force, the drag force along the Y-direction caused by the relative motion between particle and fluid critically affects the lateral migration of particles. **Figure 12** shows the distribution of the Y-component of drag force exerted on particles along the Y-direction at various axial positions. It can be seen

that the magnitude of Y-component of drag force is on the same order as that of elastic force; however, the force direction is opposite. As shown in **Figure 13**, the Y-component of drag force follows the same direction with inertial force and opposite to the elastic force. Since the inertial force is much smaller than both drag force and elastic force, it can be neglected under the conditions of Re = 0.0338, Wi = 7.926 and El = 234.273. It is worth to note that the inertial force will increase as the flow rate increases. Therefore, this model may be used to identify the critical flow rate for particle focusing in DNA solution in a microchannel.

3.2.3. Effect of DNA concentration

In this study, the main focus is on the particle focusing dynamics by using DNA as an elastic enhancer to improve the focusing efficiency. Therefore, the effect of DNA concentration on the particle focusing was investigated by the developed model. **Figure 14** gives the plots of the half-width of particle beam simulated by the CFD model along axial direction at different DNA concentrations. The simulations were carried out under the conditions of d_p = 8 μm and Q = 10 μl/h. As the DNA concentration increases from 0.5 ppm to 5 ppm, the corresponding dimensionless number Wi does not change and with the value of 7.93, while Re decreases from 0.0352 to 0.0338 and El increases from 225.03 to 234.27. Although Re and El do not differ too much from each other for the cases with different DNA concentrations, the focusing effect changes obviously (**Figure 14**). As shown in **Figure 14**, the half-width of the particle beam decreases along the axial direction for various concentrations of DNA. With the increase of the DNA

concentration from 0.5 to 5 ppm, the half-width of the particle beam throughout the whole tube drops dramatically, indicating that the DNA concentration has a sensitive effect on the particle focusing. The half-width of the particle beam decreases from 16.4 μm to 2.32μm with the increasing concentration of DNA. **Figure 15** shows the number percentage of the focused particles within ±2 μm, ±5 μm and ±8 μm of the centerline at the outlet of the tube under different DNA concentrations. It can be seen that 56% of the particles are focused within ±2 μm of the centerline at the DNA concentration of 5ppm, while only 18%, 10% and 8% of the particles focused within this range when the DNA concentrations are 2.5 ppm, 1 ppm and 0.5 ppm, respectively. Within ±5 μm of the centerline, 100% of the particles are located for the case with 5 ppm DNA concentration. 60%, 30% and 24% of the particles can be found in this range for the cases with 2.5 ppm, 1 ppm and 0.5 ppm DNA concentration. It is also observed that all the particles focused within the range ±8 μm of the centerline when the DNA concentration is 2.5 ppm. However, less than 50% of particles migrate in this range when the DNA concentration is too low, namely, 1ppm or 0.5 ppm.

3.2.4. Effect of particle diameter

Particle properties also play important roles in particle manipulation using a microfluidic device. Investigation on the effect of particle diameter can provide valuable insights into the focusing dynamics of particles. **Figure 16** shows the plot of the half-width of the particle stream along the axial direction with various particle diameters. The simulations were carried out under the conditions of C_{DNA} = 5 ppm and

Q = 10 μl/h. The corresponding dimensionless numbers *Wi*, *Re*, and *El* are 7.93, 0.0338 and 234.27, respectively. As shown in **Figure 16**, the half-width of the particle beam throughout the whole tube decreases when particle diameter changes from 1 to 10 μm, which suggests that the focusing efficiency increases with the increasing particle diameter. Larger particles tend to migrate more quickly toward the centerline of microtube as compared to smaller particles. The half-width of the particle beam decreases from 17.55 μm to 0.957 μm as the particle diameter increases from 1 μm to 10 μm, indicating that the particle size exhibits an obvious impact on the particle focusing efficiency. It can also be deduced that particle separation may be achieved with the proper design of microtube according to these characteristics. More details regarding the number percentage of the focused particles within ±2 μm, ±5 μm and ±8 μm of the centerline with different particle diameters are shown in **Figure 17**. It can be seen that 8%, 20% and 34% of the particles are focused within ±2 μm, ±5 μm and ±8 μm of the centerline respectively when the particle diameter is 1 μm. As the particle diameter increases, a higher percentage of particles can be seen within the corresponding ranges around the centerline. When the particle size increases to 5.8 μm, 100% of particles migrate to the region within ±8 μm of the centerline where 72% and 22% of the particles are located within ±5 μm and ±2 μm of the centerline. For the case with a particle diameter of 8 μm, 100% of particles focus within ±5 μm of centerline with 56% within ±2 μm. For the case with a particle diameter of 10 μm, all the particles migrate into ±2 μm of the centerline. With the developed model, the details of particle fraction at the microtube are able to be captured, which would help on the design of

microchannel or selection of particle for the application in particle focusing.

3.2.5. Effect of flow rate

Figure 18 shows the half-width of the particle beam along the axial direction with various flow rates. The simulations were carried out under the conditions of C_{DNA} = 2.5 ppm and d_p = 8 μm. As the flow rate increases from 1 μl/h to 50 μl/h, the corresponding dimensionless number *El* does not change and with the value of 229.14, while *Re* increases from 0.0035 to 0.173 and *Wi* increases from 0.793 to 39.63. As shown in **Figure 18**, the half-width of the particle beam increases with the increasing flow rate. However, only 3.23 μm increment in the half-width of particle beam at the outlet of the tube (X = 0.05 m) can be seen even when the operating flow rate is increased by 50 times (from 1 μl/h to 50 μl/h). When the flow rate is increased from 1 μl/h to 20 μl/h, the half-width of the particle beam throughout the whole tube increases slightly, indicating the less sensitive effect of the operating flow rate on particle focusing in DNA solution. In other words, a wide range of flow rate may be used to achieve particle focusing in the DNA laden fluid flow system, which is consistent with the findings of previous experimental work (*Kang et al., 2013*). Higher throughput may be achieved when the system is able to tolerate a higher flow rate with a little impact on the focusing efficiency. **Figure 19** gives the number percentage of the focused particles within ±2 μm, ±5 μm and ±8 μm of the centerline at different flow rates. As the flow rate increases, the particle number percentage within ±2 μm of the centerline almost keep constant while decreases from 64% to 46% within ±5 μm of the centerline. This indicates that

the flow rate affects the particle percentage in the region near the boundary of particle beam but hardly affects the particle percentage in the region very close (±2 μm in this study) to the centerline. The outer particles around centerline receive larger elastic force and inertial force. The elastic force is found to be the dominant force under the operating conditions in this study.

Conclusions

In this study, a CFD model was developed to investigate the particle focusing dynamics of DNA laden fluids in a microtube. Oldroyd-B constitutive equations were used to describe the flow behaviors of dilute DNA solution passing through the microtube. A 2D Lagrangian model based on Newton second law was employed to simulate the particle motion in DNA solution. Both the elastic force and inertial force were incorporated into the model by adding source terms to the conservation equations of the Lagrangian model. Good agreement between the simulation prediction and experimental data was obtained in terms of the particle focusing efficiency. Particle focusing behaviors, particle velocity and forces distributions throughout the whole tube were simulated and analyzed to investigate the particle focusing dynamics. High particle concentrations can be observed not only at the centerline region but also at the vicinity of the boundaries of the particle beam at the beginning of the focusing process. Simulation results of particle velocity distribution showed that the particle lateral migration rates at different radial positions are not a constant value and those particles far away from the centerline migrate faster than those near the centerline. The DNA

concentration and particle diameter exhibit a greater influence on the focusing efficiency while flow rate shows much less impact. The developed model in this study could serve as an effective tool to investigate the particle focusing dynamics in microchannels as well as the selection of materials for passive particle manipulations. Further, the effect of channel dimension on the particle focusing behaviors, particle velocity distribution and force distribution could be obtained for microchannel system with different configurations (length, diameter and shape), which can provide insights into the design of microfluidic devices.

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Nomenclatures

c Concentration of polymer, kg/m^3 (ppm)

c^* Overlapping concentration, kg/m^3

C_D Drag coefficient

c_{DNA} Concentration of DNA, kg/m^3 (ppm)

C_{eL} Non-dimensional elastic lift coefficient

C_{iL} Non-dimensional inertial lift coefficient

c_p Concentration of particle, µl^{-1}

D Hydraulic diameter of microchannel, m

d_p Particle diameter, m

El Elasticity number

$\vec{F}_D$ Drag force exerted on the particle, N

$\vec{F}_{eL}$ Elastic lift force, N

$\vec{F}_{iL}$ Inertial lift force, N

$\vec{F}_T$ Total force exerting on the particle, N

$\vec{n}$ Unit normal vector

N_1 First normal stress difference, Pa

P_{out} Pressure at out, Pa

Q Flow rate of suspension, µl/h

R Radius of the microchannel, m

Re Reynolds number

t Time, s

$\underline{\underline{T}}$ Extra stress contributed by the DNA, Pa

T_{11} Normal stresses in the flow translational direction, Pa

T_{22} Normal stresses in the velocity gradient direction, Pa

U Average fluid velocity at the inlet, m/s

$\vec{u}$ Velocity of partilce, m/s

u_x Velocity of partilce in the X direction, m/s

u_y Velocity of partilce in the Y direction, m/s

$\vec{v}$ Velocity of fluid, m/s

v_x Velocity of fluid in the X direction, m/s

v_y Velocity of fluid in the Y direction, m/s

Wi Weissenberg number

Greek Letters

$\dot{\gamma}$ Shear rate, 1/s

η Total viscosity of the solution, Pa·s

η_p Viscosity contributed by DNA, Pa·s

η_s Viscosity of solvent, Pa·s

λ Relaxation time of DNA, ms

μ_p Relative viscosities of the polymer, Pa·s

μ_s Relative viscosities of the solvent, Pa·s

ρ Density of DNA solution, kg/m^3

ρ_p Density of particle, kg/m^3

$\underline{\underline{\sigma}}$ Total stress, Pa

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